Trichloroacetic acid, decyl ester

Other names: Decyl trichloroacetate
Inchi: InChI=1S/C12H21Cl3O2/c1-2-3-4-5-6-7-8-9-10-17-11(16)12(13,14)15/h2-10H2,1H3
InchiKey: JVOWHDCGJSEUMO-UHFFFAOYSA-N
Formula: C12H21Cl3O2
SMILES: CCCCCCCCCCOC(=O)C(Cl)(Cl)Cl
Mol. weight [g/mol]: 303.65
CAS: 65611-33-8

Physical Properties

Property code	Value	Unit	Source
gf	-216.71	kJ/mol	Joback Method
hf	-591.78	kJ/mol	Joback Method
hfus	34.80	kJ/mol	Joback Method
hvap	63.32	kJ/mol	Joback Method
log10ws	-5.27		Crippen Method
logp	5.041		Crippen Method
mcvol	224.100	ml/mol	McGowan Method
pc	1713.19	kPa	Joback Method
rinpol	1760.00		NIST Webbook
rinpol	1762.70		NIST Webbook
rinpol	1760.00		NIST Webbook
rinpol	1762.70		NIST Webbook
rinpol	1771.00		NIST Webbook
ripol	2160.00		NIST Webbook
ripol	2160.00		NIST Webbook
tb	659.31	K	Joback Method
tc	851.10	K	Joback Method
tf	389.34	K	Joback Method
vc	0.868	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	558.87	J/mol×K	659.31	Joback Method

cpg	572.87	J/mol×K	691.27	Joback Method
cpg	586.07	J/mol×K	723.24	Joback Method
cpg	598.52	J/mol×K	755.20	Joback Method
cpg	610.24	J/mol×K	787.17	Joback Method
cpg	621.27	J/mol×K	819.13	Joback Method
cpg	631.64	J/mol×K	851.10	Joback Method
dvisc	0.0018663	Pa×s	389.34	Joback Method
dvisc	0.0009436	Pa×s	434.33	Joback Method
dvisc	0.0005423	Pa×s	479.33	Joback Method
dvisc	0.0003427	Pa×s	524.32	Joback Method
dvisc	0.0002329	Pa×s	569.32	Joback Method
dvisc	0.0001675	Pa×s	614.31	Joback Method
dvisc	0.0001260	Pa×s	659.31	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C65611338&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
gf: Standard Gibbs free energy of formation
hf: Enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hvap: Enthalpy of vaporization at standard conditions
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
pc: Critical Pressure
rinpol: Non-polar retention indices
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature

tf: Normal melting (fusion) point

vc: Critical Volume